COMPUTATIONALLY MEDIATED MICROSCOPY/MICROANALYSIS: THE NEXT FRONTIER

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Over the last three decades, microscopists and microanalysts have successfully developed, documented and exploited a large number of experimental techniques for the characterization of the morphology, crystallography, elemental, chemical and electronic structure of their samples. While the application of any of these now “routine” tools of microcharacterization remains the foundation of the work reported in the microscopy or microanalysis literature, it can be safely asserted that the technologically important problems of the next decade will demand an ever increasing sophistication in how we attack and solve the ensuing generation of problems using the resources we have at hand. It is also reasonably safe to say that while improving something as basic as the resolution of an instrument will generally facilitate studying a new class of materials, it will not fundamentally change how we work, it will only change what one studies. To truly create a new paradigm of how we, as experimentalists, enlist resources to solve vexing problems; we have to step back and consider what are all the limiting factors to employing our resources to their greatest utility, then we must come up with new ways of combining these resources to change the how we might tackle new problems.

Assuming, therefore, that we are interested in extending the range and diversity of problems that we will be dealing with in the future then we will be challenged to undertake experimental measurements which here-to-for were considered beyond the realm of achievability. The obvious questions become: In what way are our current experiments limited by the way we work? How can we push the envelope of technology to permit our solving new types of problems? Where will the breakthroughs in new ways of working be realized? Given the ever growing tendency to add computational resources to our instruments it is clear that the next advance will be directly related to how well we can effectively tie the realms of computational science and experimental science together. In the past we have used computers to simply speed up our experiments, in the last decade we have expanded this role to permit various degrees of telepresence operation[1] and/or automation. In the coming decade the key to changing how we work will be to realize that once an effective interface of instrumentation and computational tools has been developed, then we must change the way in which we design and conduct our experiments. This means re-examining how we do experiments so that measurements are done not just quickly, but rather, in such a way so as to maximize the information measured from the specimen. In this way the data acquired can be “mined” for content after the fact, using tools which may not reside within the instrument room, but at remote locations and not just by the instrument operator but a colleague from any location.

As example of this new type of experiment consider the technique of Position Resolved Diffraction[2] which is currently being used at ANL for the study of nanoscale magnetic structures. Here a focused electron probe is sequentially positioned in a two dimensional pattern on a thin TEM specimen and at each point a complete electron diffraction pattern (EDP) is acquired, stored and analyzed. Determination of the spatial variation in the diffraction pattern at individual points on the sample allows scientists to study the subtle changes resulting from differences due to ferromagnetic/electric domain formation and motion. In the past this type of experiment would have been simply dismissed as impractical. Why? It simply puts too great an onus on the operator facilitate the experiment. A minimal scoping study measurement involves measurement on a 64 x 64 pixel spatial array (X,Y) grid at each point measuring a diffraction pattern at 1K x 1K pixels (α x β) yielding ~ 4Gbytes of data per measurement. Extending this experiment to arrays of dimensions of (512 x 512) yields ~ 275 Gbytes of data, while a study of 1K x 1K array of points produces ~ 1Tbyte of data. Both the former and later of these scenarios is well beyond the current processing capabilities of any humanly directed process, as well as for most existing desktop DAQ systems present on instruments today.

The challenge to the next generation of investigations thus becomes integrating new advances in information technology, networking, and processing with our methodology in such a way that we can realistically tackle this new generation of data intensive experiments. These new types of studies will be poised to tackle the forefront problems and scientific challenges which await our scrutiny. To achieve this goal, we are developing a set of Grid[2] enabled tools to facilitate network coordination of computational resources with the aim of changing the way experiments are done. The intention is for these new tools to integrate network aware resources linking: storage, communication, control together with computational power to facilitate not only data acquisition, but also data mining and remote collaboration to a degree which is unprecedented today[3-4]
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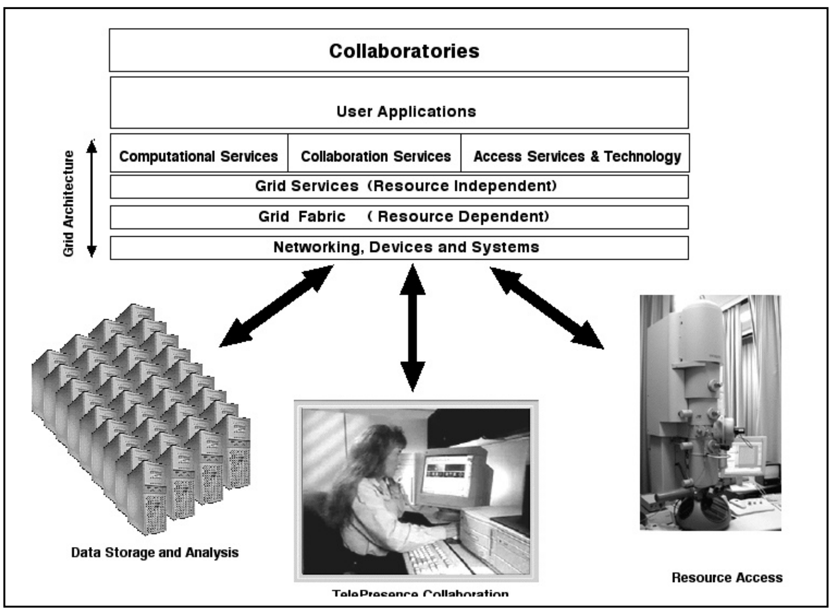

Figure 1. Linking Collaboratories, User Applications and Grid Technologies/Services for state-of-the-art Microscopy and Microanalysis.

References:

1.) M.A. O'Keefe, "Experiences with Remote Microscopy" , these proceedings.
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3.) K. Czajkowski,etal. Proc. of the 10th IEEE Int. Symp. on HPDC IEEE Press, August 2001."Grid Information Services for Distributed Resource Sharing"

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